

Adiabatic connection between the RVB State and the ground state of the half filled periodic Anderson model

K. Kimura^{1*}, Y. Hatsugai², and M. Kohmoto¹

¹*Institute for Solid State Physics, University of Tokyo, 7-22-1, Roppongi, Minato-ku, Tokyo 106, Japan*

²*Department of Applied Physics, University of Tokyo, 7-3-1, Hongo, Bunkyo-ku, Tokyo 113, Japan*

Abstract

A one-parameter family of models that interpolates between the periodic Anderson model with infinite repulsion at half-filling and a model whose ground state is exactly the Resonating-Valence-Bond state is studied. It is shown numerically that the excitation gap does not collapse. Therefore the ground states of the two models are adiabatically connected.

I. INTRODUCTION

Recently correlation effects in electronic systems have been focused and studied extensively. This is an old problem, however, it still is supplying interesting new physics both experimentally and theoretically.

One can classify the ground states of strongly correlated systems into two. The one is a metallic state which have a gapless excitation. The Fermi-liquids and the Tomonaga-Luttinger liquids in one-dimension are in this class. The other is an insulator which has a finite excitation gap. A simple example is a band insulator. Also there is another type of insulators which are caused by correlation (Mott-insulators). A well-known example of the correlated insulators is the half filled Hubbard model in one dimension.

Another example with the correlation gap is an energy gap of the half-filled Kondo lattice in one dimension. The charge degree of freedom on the sites with on-site Coulomb repulsion are frozen. In this model both the charge and the spin degree of freedom have a finite excitation gap though the lowest one is the spin excitation [1]. The periodic Anderson model which we investigate is a model where the charge degree of freedom are also active.

Principle of adiabatic continuation is important in condensed matter physics. For example, the basic assumption of the Fermi liquid theory is that the interacting system with quasiparticles is adiabatically connected to the non-interacting system with several phenomenological parameters. More specifically, the non-interacting fermions has one to one correspondence to the quasiparticle of the interacting electrons and there are no gap closing in the process of increasing the interaction from zero to reach the interacting model. Another notable example is the theory of the fractional quantum Hall effect. The adiabatic transformation in which the external magnetic fluxes are put on the electrons to become bosons [2] or composite fermions [3] is the crucial assumption.

In this paper we choose the model of Strack [4] in one dimension as the canonical system with the correlation gap. The ground state is exactly the Resonating-Valence-Bond (RVB) state [4-8]. See, *e.g.*, Ref.9 for the form of the RVB state. In this model, some of the correlation functions are obtained exactly [7,8]. Moreover it is connected to the periodic Anderson model in one dimension as a parameter is varied. The periodic Anderson model has been commonly used to describe the correlation effects in heavy fermion compounds and it reduces to the Kondo lattice model when the valence fluctuation is prohibited [1]. In order to clarify the relation between the two model we numerically obtain the ground state energy and the excitation gap for intermediate Hamiltonians.

II. MODELS

The Hamiltonian of the Strack model is

$$H_{ST} = \wp \sum_{n,\sigma} \{ (-\lambda_1 \lambda_2 c_{n+1,\sigma}^\dagger c_{n,\sigma} - \lambda_1 c_{n+1,\sigma}^\dagger f_{n,\sigma} - \lambda_2 c_{n,\sigma}^\dagger f_{n,\sigma} + h.c. + \epsilon^c c_{n,\sigma}^\dagger c_{n,\sigma} + \epsilon^f f_{n,\sigma}^\dagger f_{n,\sigma}) \} \wp, \quad (1)$$

where n is an index of the unit cell. In Fig.1(a), the lattice structure of the model is shown where \circ and \bullet denote f - and c - sites respectively. Electrons at f -sites feels infinitely large

on-site Coulomb repulsion($U = \infty$) and c -sites do not have Coulomb repulsion($U = 0$). The projection operator \wp represents to project out the states with doubly occupancy at the f -sites. When one imposes $\epsilon^c = 2 - (\lambda_1^2 + \lambda_2^2)$, and $\epsilon^f = 2 - 2 = 0$, the ground state at half-filling is explicitly written

$$\begin{aligned} |\Phi_G\rangle &= \wp \prod_{n,\sigma} (\lambda_1 c_{n,\sigma}^\dagger + \lambda_2 c_{n+1,\sigma}^\dagger + f_{n,\sigma}^\dagger) |0\rangle. \\ &= \prod_n (\lambda_1 \lambda_2 d_{c_n, c_{n+1}}^\dagger + \lambda_1^2 d_{c_n, c_n}^\dagger \\ &\quad + \lambda_2^2 d_{c_{n+1}, c_{n+1}}^\dagger + \lambda_1 d_{c_n, f_n}^\dagger + \lambda_2 d_{f_n, f_{n+1}}^\dagger) |0\rangle, \end{aligned} \quad (2)$$

where

$$d_{\alpha_i, \beta_j}^\dagger = \begin{cases} \alpha_{i,\uparrow}^\dagger \beta_{j,\downarrow}^\dagger + \alpha_{j,\uparrow}^\dagger \beta_{i,\downarrow}^\dagger & \text{for } i \neq j \\ \alpha_{i,\uparrow}^\dagger \alpha_{i,\downarrow}^\dagger & \text{for } i = j \end{cases}. \quad (3)$$

Thus it is given by creations of nearest-neighbor singlet pairs on the vacuum. This state is the RVB state which we use as the canonical ground state with the correlation gap.

The existence of the finite energy gap has not been shown analytically. But it is numerically confirmed in the present work. This is consistent with the behavior of correlation functions of a local quantities which are analytically shown to be exponentially decaying [7,8]. One can expect that the excitation above the ground state is closely related to a local singlet-triplet excitation which apparently has a finite energy cost.

The Hamiltonian of the periodic Anderson model is written

$$\begin{aligned} H_{PA} &= t \sum_{n,\sigma} (c_{n+1,\sigma}^\dagger c_{n,\sigma} + h.c.) + V \sum_{n,\sigma} (c_{n,\sigma}^\dagger f_{n,\sigma} + h.c.) + \\ &\quad \epsilon^f \sum_{n,\sigma} f_{n,\sigma}^\dagger f_{n,\sigma} + U \sum_n f_{n,\uparrow}^\dagger f_{n,\uparrow} f_{n,\downarrow}^\dagger f_{n,\downarrow}, \end{aligned} \quad (4)$$

where U is the on-site Coulomb repulsion on f -sites. We consider the strong coupling limit $U \rightarrow \infty$.

These two Hamiltonians (1) and (4) is connected by changing hopping elements of the Strack model as shown in the Fig.1(c).

The intermediate Hamiltonian we study is

$$\begin{aligned} H_C &= \wp \sum_{n,\sigma} [(t c_{n+1,\sigma}^\dagger c_{n,\sigma} + t_1 c_{n+1,\sigma}^\dagger f_{n,\sigma} + t_2 c_{n,\sigma}^\dagger f_{n,\sigma} + h.c.) \\ &\quad + \epsilon^c c_{n,\sigma}^\dagger c_{n,\sigma} + \epsilon^f f_{n,\sigma}^\dagger f_{n,\sigma}] \wp. \end{aligned} \quad (5)$$

The Strack Hamiltonian (1) which is given by setting t_1 and t_2 as $t = -\lambda_1 \lambda_2$, $t_1 = -\lambda_2$, $t_2 = -\lambda_1$. Also when $t_1 = 0$, it reduces to the periodic Anderson model (4) with $U = \infty$.

III. NUMERICAL RESULTS

To calculate the ground states and the energy gaps for sufficiently large systems, we used the White's method (DMRG) [10,11]. Also numerical diagonalizations was performed for

relatively small systems to check the validity of the DMRG results. It is interesting to note that DMRG is exact in the Strack model [13]. This fact supports the locality of the RVB state.

First we start with the Strack model by setting $t = t_1 = t_2 = -1$ and $\epsilon^c = \epsilon^f = 0$ in (5). Then it is identical to the Strack's Hamiltonian (1) with $\lambda_1 = \lambda_2 = 1$. By changing t_1 while keeping the other parameters fixed in H_C , one gets the periodic Anderson model with $\epsilon^f = 0$ when $t_1 = 0$.

The excitation gap obtained numerically are plotted in Fig. 2. It interpolates $t_1 = -1$ (the Strack model) and $t_1 = 0$ (the periodic Anderson model). We used a periodic boundary condition and each values are calculated by taking an extrapolation to the infinite system size. As a reference, the energy gap obtained by the slave boson method is also plotted [13].

The system size dependence of the energy gap is shown in Fig.3 with the results with open boundary condition of the periodic Anderson model ($t_1 = 0$ in (5))

As shown in Fig.2, the excitation gap of the half-filled periodic Anderson model is connected to that of the Strack's model without gap closing. It implies that the ground state of the periodic Anderson model at half filling may have close connection to that of the RVB state. For example, both ground states are singlet and have local nature. The excitations are expected to be closely related to local singlet-triplet excitations

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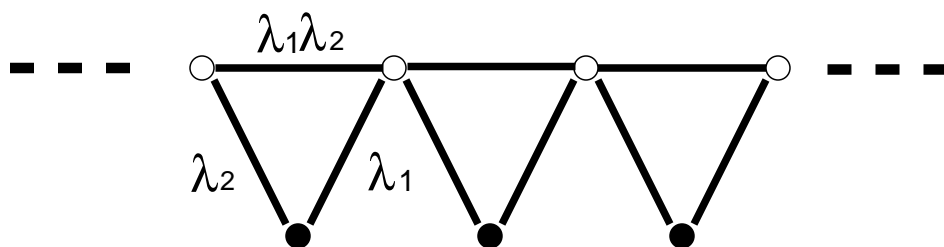
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FIGURES

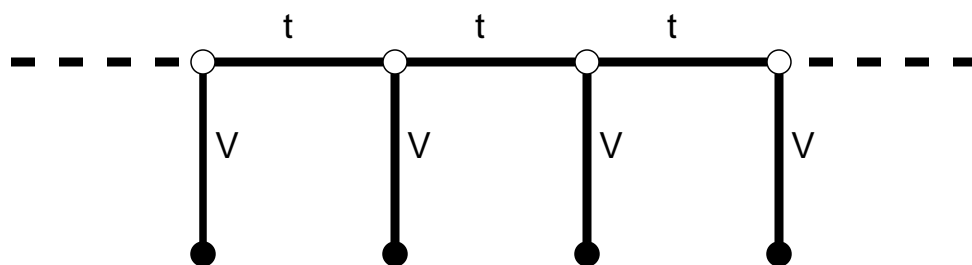
Fig. 1 Lattice structure :(a) The Strack model, (b) the periodic Anderson model, and (c) an intermediate model connecting (a) and (b).

Fig. 2 Excitation gap versus t_1 .

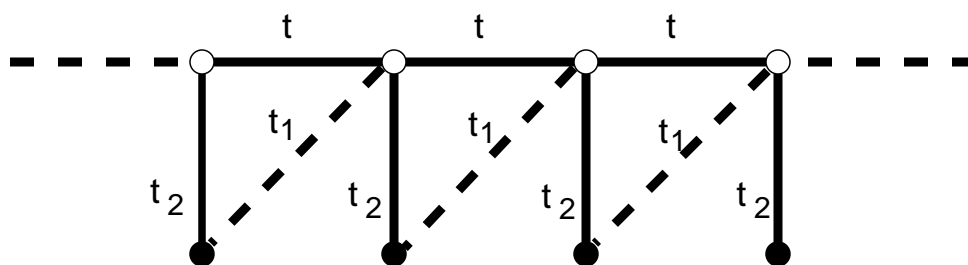
Fig. 3 Excitation gap versus $1/L$: L is the system size.



(a)



(b)



(c)

Fig.1

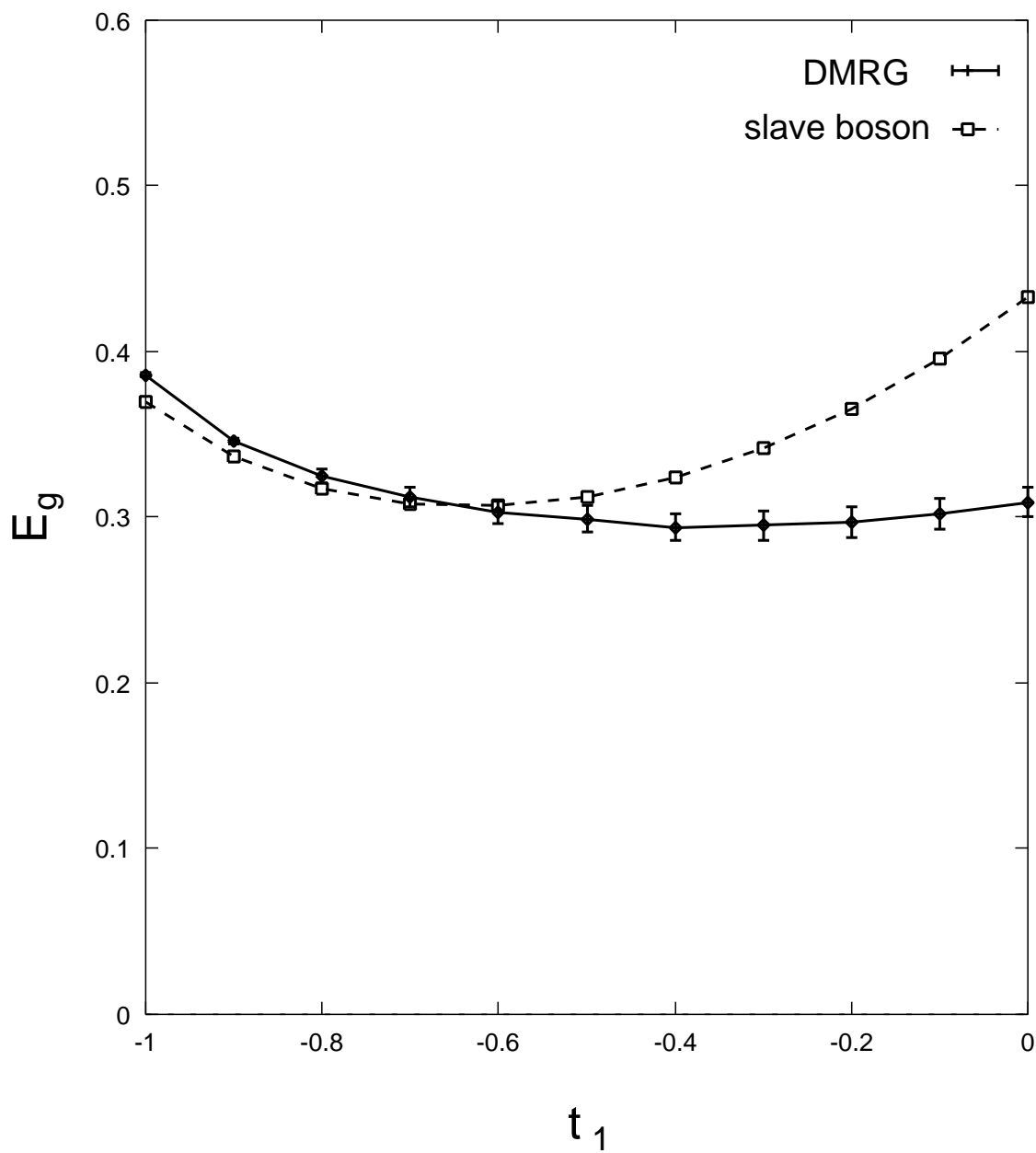


Fig. 2

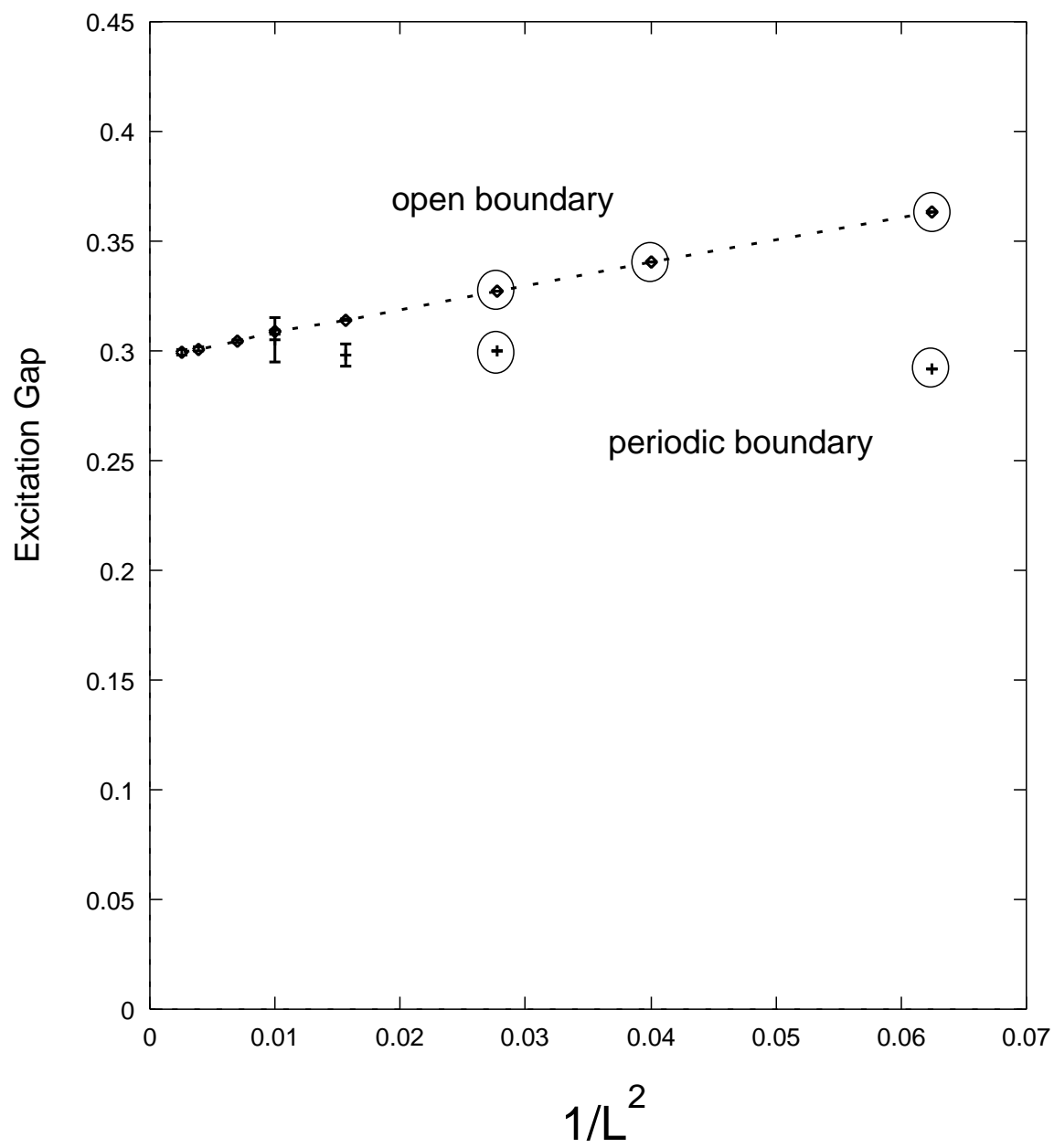


Fig. 3